

# Hubbard-Thomas-Fermi Theory of Transition Metal Oxide Heterostructures

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## Abstract

We demonstrate that the charge distributions in Hubbard-model representations of transition metal oxide heterojunctions can be described by a Thomas-Fermi theory in which the energy is approximated as the sum of the electrostatic energy and the uniform three-dimensional Hubbard model energy per site at the local density equals to a constant. When charged atomic layers in the oxides are approximated as two-dimensional sheets with uniform charge density, the electrostatic energy is simply evaluated. We find that this Thomas-Fermi theory can reproduce results obtained from full Hartree-Fock theory for various different heterostructures. We also show explicitly how Thomas-Fermi theory can be used to estimate some key properties qualitatively.

*Key words:* Mott Insulator; Heterostructure; Transition Metal Oxide; Interface

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Recent advances in techniques for layer-by-layer growth of transition metal oxides promise new types of heterostructures between strongly-correlated materials [1,2,3] and has motivated many theoretical studies devoted to exploring their physical properties [4,5,6] using simple Hubbard models augmented by a long-range Coulombic interaction term. The charge distribution near a the transition metal oxide heterostructures (TMOHs) is usually studied using Hartree-Fock theory or dynamical mean-field theory with satisfactory results. We have found that the same results can be reproduced much more simply using a Thomas-Fermi theory (TFT) in which all energy contributions other than the electrostatic one are approximated by a local density approximation [5,6]. In this paper, we derive TFT specifically for the generalized Hubbard models of TMOHs from general consideration and demonstrate how it can be used to estimate some key properties of the TMOHs.

The simplest toy model to investigate the TMOHs is:  $H = H_U + H_C$ , where  $H_U$  is the single-band Hubbard model describing on-site correlations and  $H_C$  is the long-ranged Coulomb interaction. Following the spirit of TFT, we can write down TF equation as:

$$\mu(\rho(\vec{r})) + v_H(\vec{r}) = \text{const.} \quad (1)$$

where  $\mu(\rho)$  and  $v_H(\vec{r})$  are the chemical potential of the Hubbard model for a uniform system with density  $\rho$  and

the electrostatic potential at position  $\vec{r}$ . Since the transition metal oxides have a natural layered structures, we allow the average density to vary from layer to layer near the heterojunction. It is usually a good approximation to ignore the periodic but non-uniform density variation within each layer in calculating the electrostatic potential. In this approximation both  $\mu(\vec{r})$  and  $v_H(\vec{r})$  depend only on the position along the growth direction  $\hat{z}$  and the TF equation reduces to:

$$\mu(\rho(z)) + v_H(z) = \text{const.} \quad (2)$$

where  $\rho(z)$  is the average electron density at  $z$ .

The electrostatic potential  $v_H$  can be evaluated from self-consistently determined densities by solving the Poisson equation. In the continuum limit each layer can be considered as a two-dimensional sheet with uniform effective charge density  $\sigma$ . Consequently, the electrostatic potential at  $z$  is contributed by all charged layers at  $z'$  with effective charge density  $\sigma(z')$ :

$$v_H(z) = \sum_{z'} v_H(z', z) = 2\pi U_c \sum_{z'} \sigma(z') |z - z'| \quad (3)$$

where  $U_c = e^2/\epsilon a$  is the strength of long-ranged Coulomb interaction, and  $a$  is the lattice constant. The next thing is to evaluate the chemical potential  $\mu(\rho(z))$ . Ideally  $\mu(\rho(z))$  should be obtained from exact results for the homogeneous three-dimensional Hubbard model. Since this is not available some approximations are required. The simplest choice is the Hartree-Fock approximation.

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Since Hartree-Fock theory can have separate solutions for antiferromagnetic (AFM) and ferromagnetic (FM) states (among others), we can solve TF equation for both cases. It has been shown that TFT accurately reproduces the charge distribution along the growth direction obtained by Hartree-Fock theory for modulation-doped Mott-insulator-Mott-insulator and Mott-insulator-band-insulator heterostructures[5].

Recently the authors proposed that electronic interface reconstruction (EIR), a charge transfer from the outmost surface layer to the interface, can occur in a polar ( $AMO_3$ )-nonpolar ( $A'M'O_3$ ) perovskite Mott-insulator heterostructure[6]. The effective charge densities are  $\sigma = 1$  for the  $AO$  layers, 0 for  $A'O$  layers,  $\rho(z)$  for the  $MO_2$  layers, and  $(\rho(z) - 1)$  for  $M'O_2$ , where  $\rho(z)$  is the average electron density on the  $d$ -band of transitional metal ions  $M(M')$ . We consider a film with  $N_p$  pairs of  $AO - MO_2$  layers and  $(N - N_p)$  pairs of  $A'O - M'O_2$  layers. The electrostatic potential for this case is[6]:

$$\frac{v_H(z)}{2\pi U_c} = \sum_{z_A} |z - z_A| - \sum_{z' \neq z} [\rho(z') - \theta(z' - N_p)] |z' - z| \quad (4)$$

where  $z_A = 1.5, 2.5, \dots, N_p + 0.5$ ,  $(z, z') = 1, 2, \dots, N$ , and  $\theta(z' - N_p)$  is the Heaviside step function. The charge distribution calculated from TFT is given in Fig.1, and is nearly identical to the results of Hartree-Fock theory presented in the Fig. 2(b) of Ref[6]. The success of TFT for different TMOHs is remarkable. The critical reason for this success is that the charge distribution in these TMOHs is a consequence of competition between the on-site correlation energy (represented by  $\mu(\rho(z))$ ) and the spatial long-ranged Coulomb field (represented by  $v_H(z)$ ), and these two dominant energy scales are correctly captured by TFT. This feature also promises that if the chemical potential  $\mu(\rho(z))$  can be obtained more realistically by some sophisticated approaches for the homogeneous three-dimensional Hubbard model, TFT can also predict the correct charge distribution for most TMOHs without heavy computation.

Another advantage of TFT emerges if we want to estimate some key properties qualitatively. It is known, for example[6], that a minimum value of  $N_p$  is required for EIR to occur. This minimum value can be estimated easily using TFT. Since only the outer most surface and the interface layer have electron densities different from 1 when EIR first occurs, we consider:

$$\mu_{U_1}(\rho(z_1)) + v_H(z_1) = \mu_{U_2}(\rho(z_i)) + v_H(z_i) \quad (5)$$

where  $z_1 = 1$  is the position of outmost layer and  $z_i = N_p + 1$  is that of doped interfacial layer by our convention.  $U_1$  ( $U_2$ ) is the Hubbard  $U$  parameter for polar (nonpolar) material. We put  $\rho(z_1) = 1 - x$ ,  $\rho(z_i) = 1 + x$ , and  $\rho(z) = 1$  for all other values of  $z$ , then we can evaluate  $v_H(z_1)$  and  $v_H(z_i)$ :

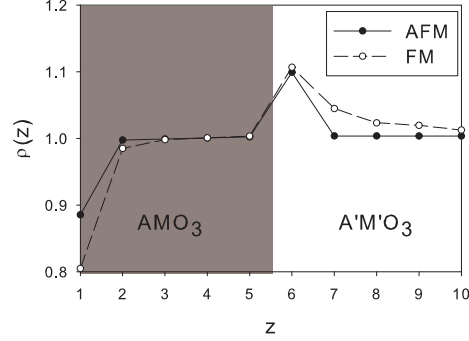


Fig. 1. Electron distribution calculated by TFT for AFM and FM states with  $U_1/t = U_2/t = 20$ ,  $U_c = 0.8$ ,  $N_p = 5$ , and  $N = 10$  for a polar ( $AMO_3$ )-nonpolar ( $A'M'O_3$ ) heterostructure.

$$\begin{aligned} \frac{v_H(z_1)}{2\pi U_c} &= \sum_{z_A} |z_1 - z_A| - \sum_{z'=2}^{N_p} |z' - z_1| - x|z_i - z_1| \\ \frac{v_H(z_i)}{2\pi U_c} &= \sum_{z_A} |z_i - z_A| - \sum_{z'=2}^{N_p} |z' - z_i| - (1-x)|z_i - z_1| \end{aligned} \quad (6)$$

It is straightforward to compute:  $\sum_{z_A} |z_1 - z_A| = \sum_{z_A} |z_i - z_A| = \frac{N_p^2}{2}$ ,  $\sum_{z'=2}^{N_p} |z' - z_1| = \sum_{z'=2}^{N_p} |z' - z_i| = \frac{N_p^2 - N_p}{2}$ , and  $|z_i - z_1| = N_p$ . So if we require  $x \geq 0$ , we find  $N_p$  should be:  $N_p \geq \frac{\mu_{U_2}(1^+) - \mu_{U_1}(1^-)}{2\pi U_c}$ . The insight revealed by this expression has been discussed in Ref[6]. A similar analysis has been discussed earlier[5].

In summary, we have derived a TFT appropriate for Hubbard model descriptions of TMOHs and applied it to cubic perovskite heterojunction systems. We have shown that this TFT can be used in an appropriate way to estimate some key properties which are difficult to treat analytically in Hartree-Fock theory and dynamical mean-field theory. The applicability of TFT indicates that the on-site correlation and long-ranged Coulomb interaction are the most dominant energy scales in TMOHs. For this reason it is possible to create new types of two-dimensional systems which inherit strong-correlation features from the Mott insulator near interface between TMOs.

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